

```

library("reticulate")
library("fanplot")
np <- import("numpy")
ntimepts <- 1000
burn_in_n <- 1e3
skip <- 10
home_directory <- "/Users/aarcher/PycharmProjects/13_PDO_Pathway_Inference/MCMC/"
directory <- paste(home_directory,"output/MCMC_results_formatted/adaptive/preset_std/lambda_0,01_beta_0"
directory_plot <- paste(home_directory,"output/MCMC_results_plots/adaptive/preset_std/lambda_0,01_beta_0

library(readr)
time_series_df <- read_csv("~/PycharmProjects/13_PDO_Pathway_Inference/data/data_files/data_time_series.csv")

## Rows: 31 Columns: 5

## -- Column specification -----
## Delimiter: ","
## dbl (5): Glycerol Init (g/L), Time (hrs), Glycerol (mM), PDO (mM), DCW (g/L)

##
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this message.

MBC = 8.5 #TODO double check this value
MIC= 1.5 #TODO double check this value
ln = c(5, 20, 50, 80, 95)

for(gly_cond in c(50,60,70,80)){
  #data points
  rows_bool = time_series_df$`Glycerol Init (g/L)` == gly_cond
  time_samples = time_series_df[rows_bool,]$`Time (hrs)`
  time_disc = seq(0,max(time_samples),length.out=ntimepts)
  gly_samples = time_series_df[rows_bool,]$`Glycerol (mM)`
  pdo_samples = time_series_df[rows_bool,]$`PDO (mM)`

  #solutions evaluated parameter points
  data_set <- np$load(paste(directory,'/solution_array_burn_in_',burn_in_n,'_skip_', skip,'_ntimepts_',gly_cond,'.npz'))
  #TODO add in experimental points
  #TODO add in time axis
  #TODO in time series of median parameter
  #TODO add in time series of mean parameter
  filter <- rowSums(data_set[,6] < data_set[1,1,4]) == 1000 #TODO compare the entire row to each column
  data_set <- data_set[filter,,]
  #png(file=paste(directory_plot,'data_distribution_GLY_ext_',gly_cond,'_fan_plot.png',sep=''))
  fan0(data=data_set[,4],xlim=c(0,max(time_samples)),ylim=c(0,max(data=data_set[,4])),ylab='External glycerol concentration (mM)')
  points(time_samples,gly_samples,pch=16)
  median_gly <- apply(data_set[,4], 2, median, na.rm=T)
  lines(time_disc,median_gly,lty=2)
  legend(x="topright", legend=c("median model result","experimental observations"), lty=c(NA,2), pch=c(16,1))
  title('Time series distribution of \n external glycerol concentration (mM)')
  #dev.off()
  #png(file=paste(directory_plot,'data_distribution_13PDO_ext_',gly_cond,'_fan_plot.png',sep=''))
  plot.new()
  #par(mar=c(5.1, 6.1, 4.1, 2.1))
}

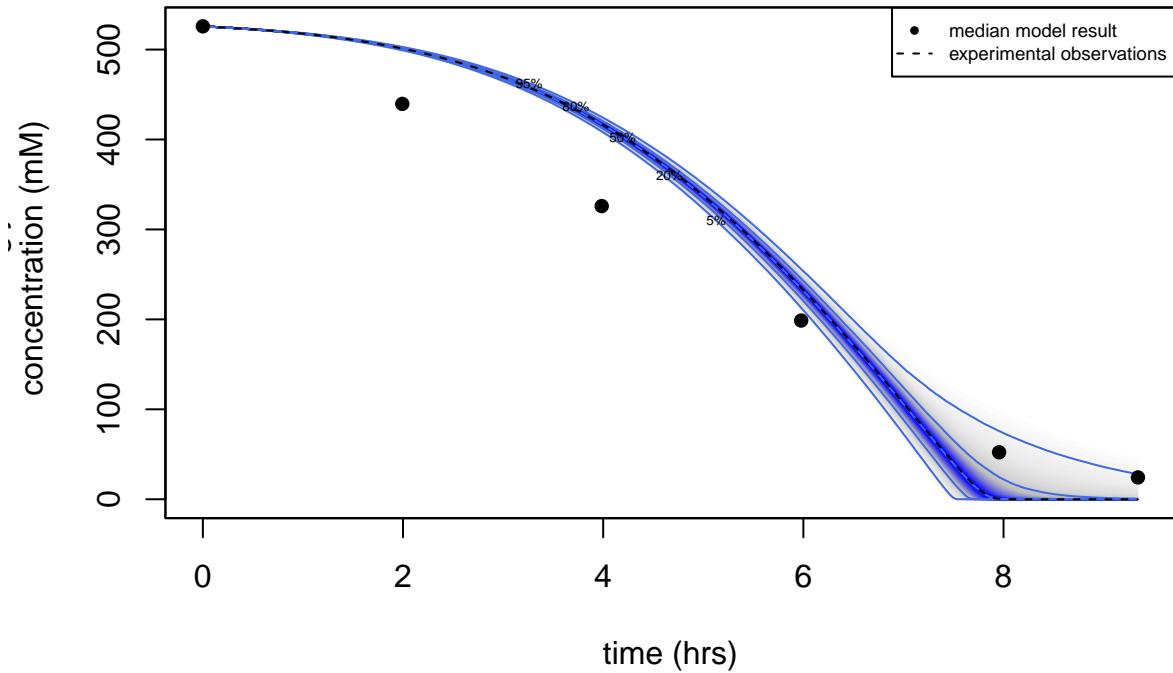
```

```

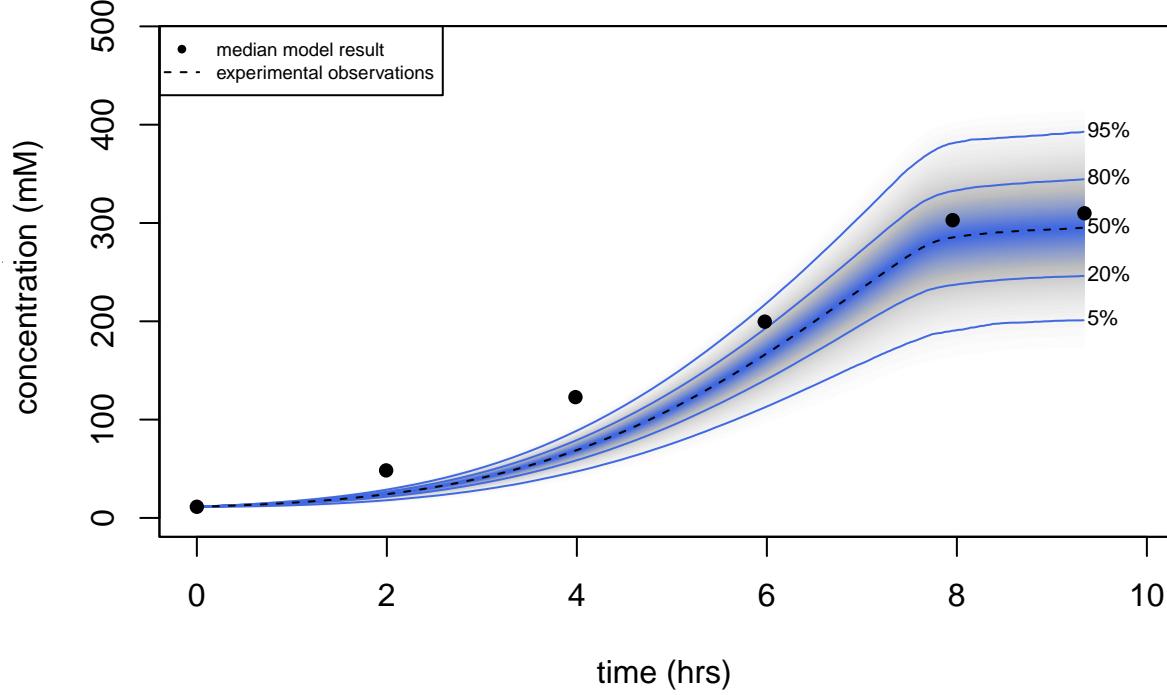
fan0(data=data_set[,6],xlim=c(0,max(time_samples)+0.5),ylim=c(0,max(data=data_set[,6])),ylab='External 1,3-PDO concentration (mM)')
title('Time series distribution of \n external 1,3-PDO concentration (mM)')
points(time_samples,pdo_samples,pch=16)
median_pdo <- apply(data_set[,6], 2, median, na.rm=T)
lines(time_disc,median_pdo,lty=2)
legend(x="topleft", legend=c("median model result","experimental observations"), lty=c(NA,2), pch=c(16,2))
#dev.off()
#png(file=paste(directory_plot,'data_distribution_3HPA_cyto_',gly_cond,'_fan_plot.png',sep=''))
HPA_data_set <- pmax(data_set[,2],10^(-10))
log_HPA_data_set <- log10(HPA_data_set)
median_log_HPA <- apply(log_HPA_data_set, 2, median, na.rm=T)
plot.new()
#par(mar=c(5.1, 6.1, 4.1, 2.1))
fan0(data=log_HPA_data_set,xlim=c(0,max(time_samples)),ylim=c(min(log_HPA_data_set),max(data=log_HPA_data_set)))
title('Time series distribution of \n cytosolic 3-HPA concentration (mM)')
lines(time_disc,median_log_HPA,lty=2)
legend(x="topright", legend=c("median model result"), lty=c(2), pch=c(NA),cex=0.6)
#dev.off()
# TODO add in quantile ranges
#TODO add line with MIC
#png(file=paste(directory_plot,'data_distribution_3HPA_MIC_MBC_cyto_',gly_cond,'_fan_plot.png',sep=''))
#par(mar=c(5.1, 6.1, 4.1, 4.1))
fan0(data=log_HPA_data_set,xlim=c(0,max(time_samples)),ylim=c(min(log_HPA_data_set),log10(50)),ylab='Cytosolic 3-HPA concentration (mM)')
abline(h=log10(MIC), lty=2)
abline(h=log10(MBC), lty=2)
axis(4, at=c(log10(MIC),log10(MBC)),labels=c('MIC','MBC'), las=2,cex.axis=0.79)
title('Time series distribution of \n cytosolic 3-HPA concentration (mM)')
lines(time_disc,median_log_HPA,lty=2)
legend(x="topright", legend=c("median model result"), lty=c(2), pch=c(NA),cex=0.6)
#dev.off()
# TODO add in quantile ranges
#TODO add line with MBC
}

```

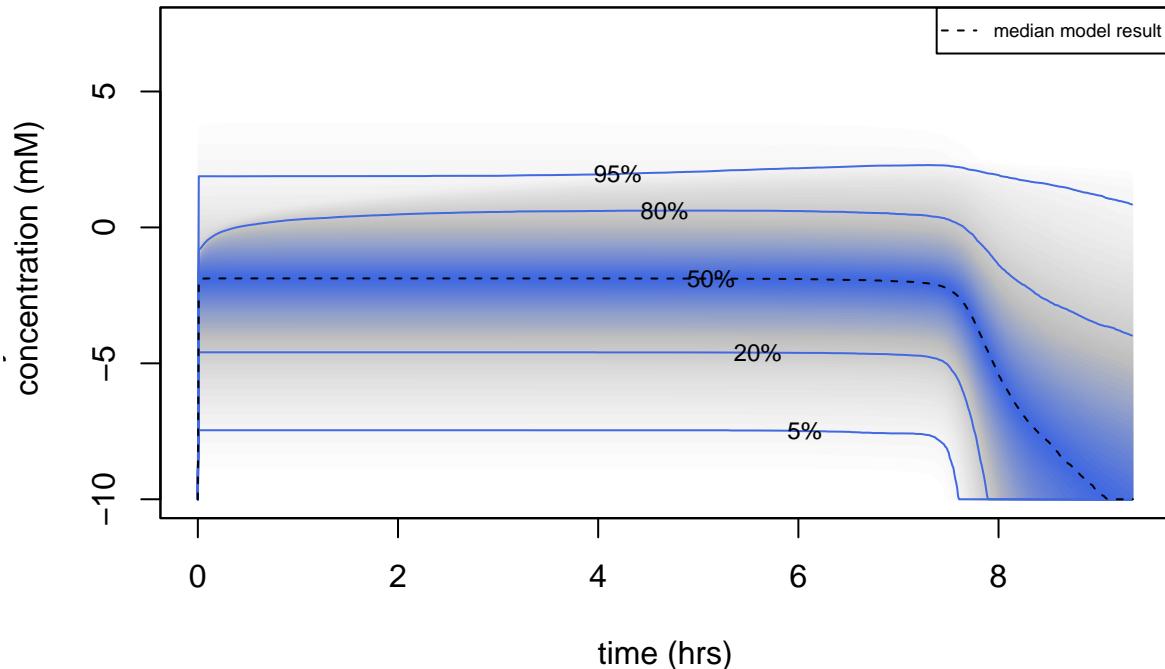
Time series distribution of external glycerol concentration (mM)



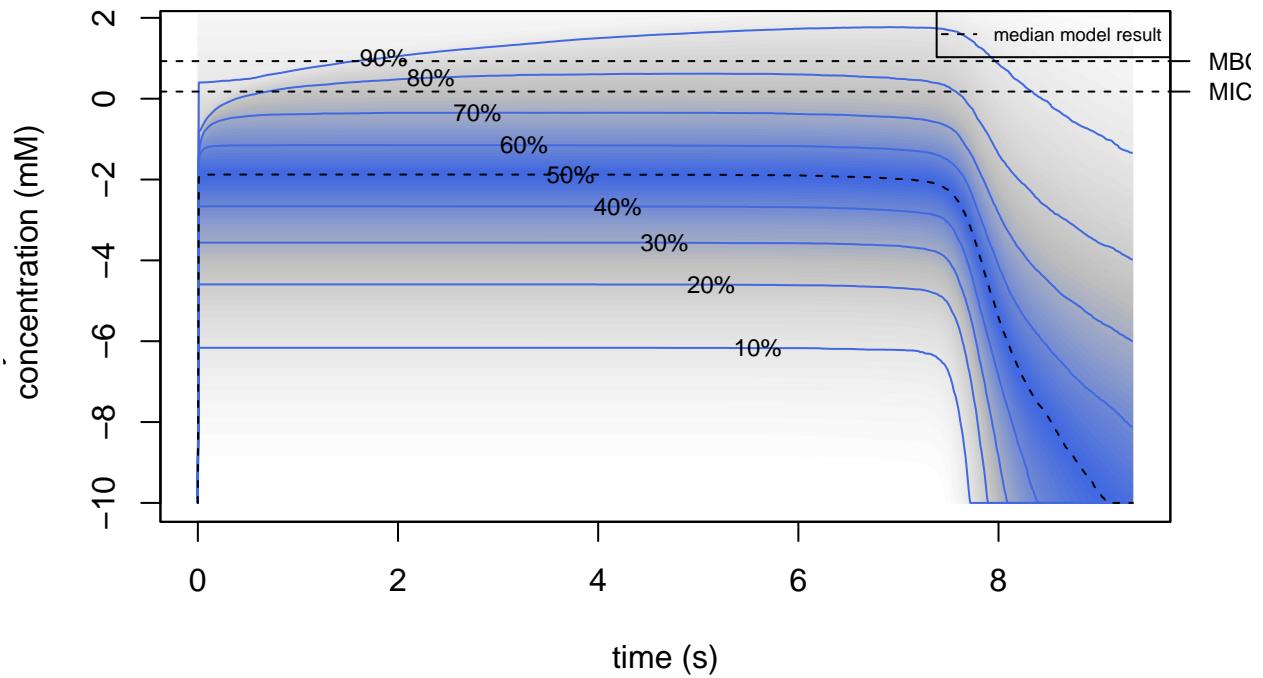
Time series distribution of external 1,3-PDO concentration (mM)



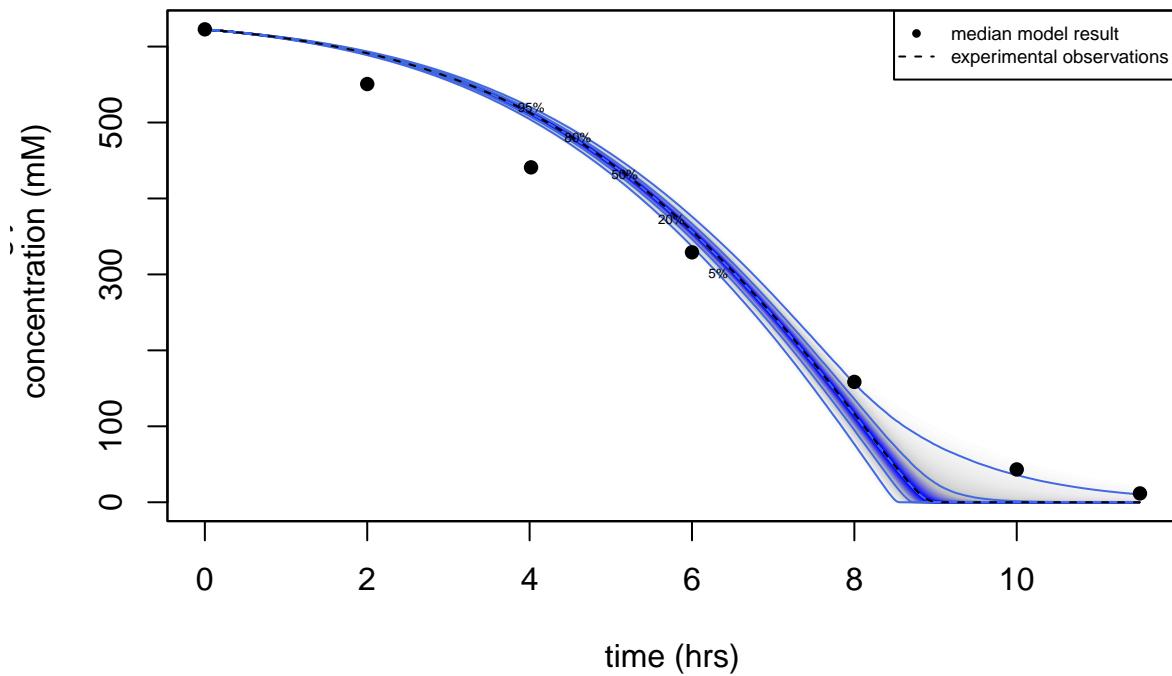
Time series distribution of cytosolic 3–HPA concentration (mM)



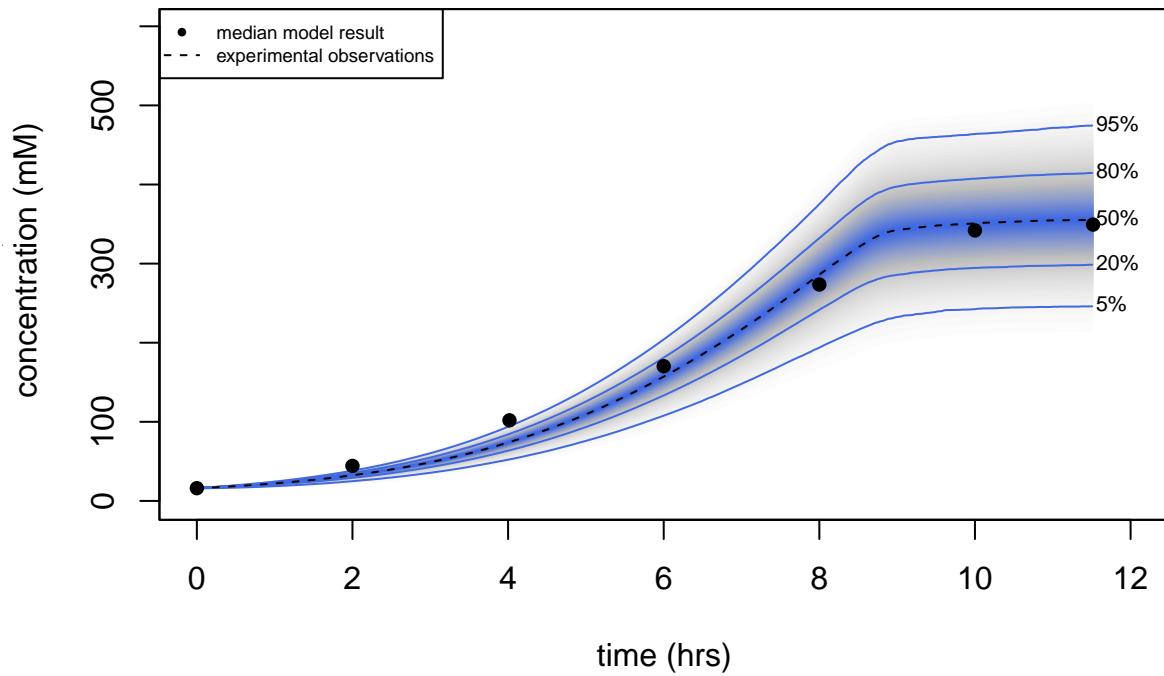
Time series distribution of cytosolic 3–HPA concentration (mM)



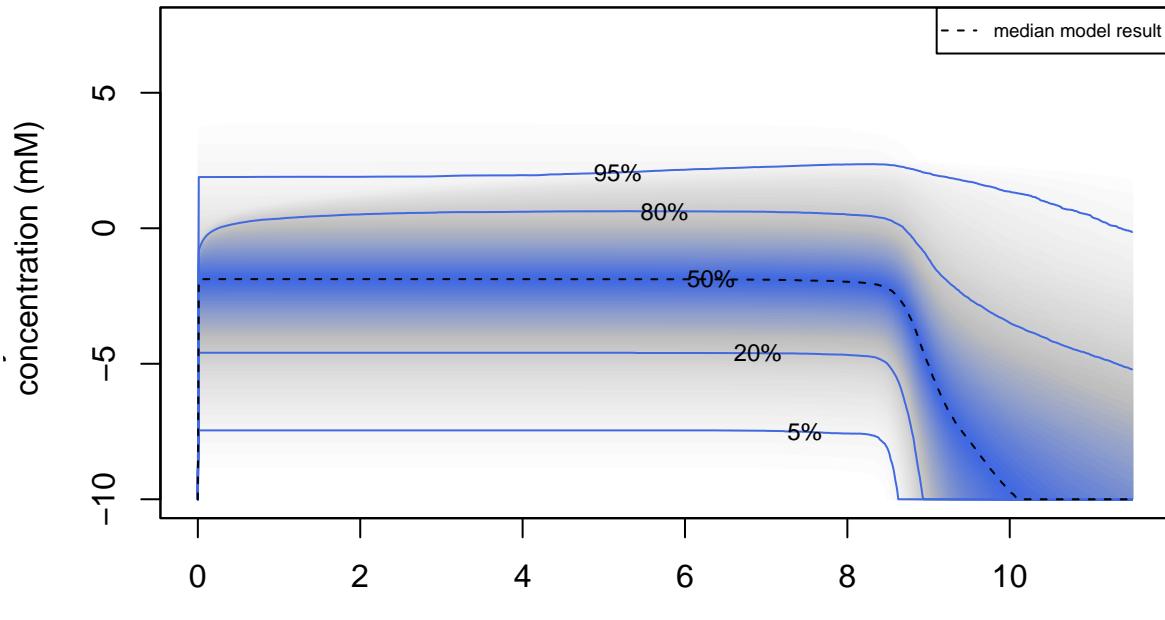
Time series distribution of external glycerol concentration (mM)



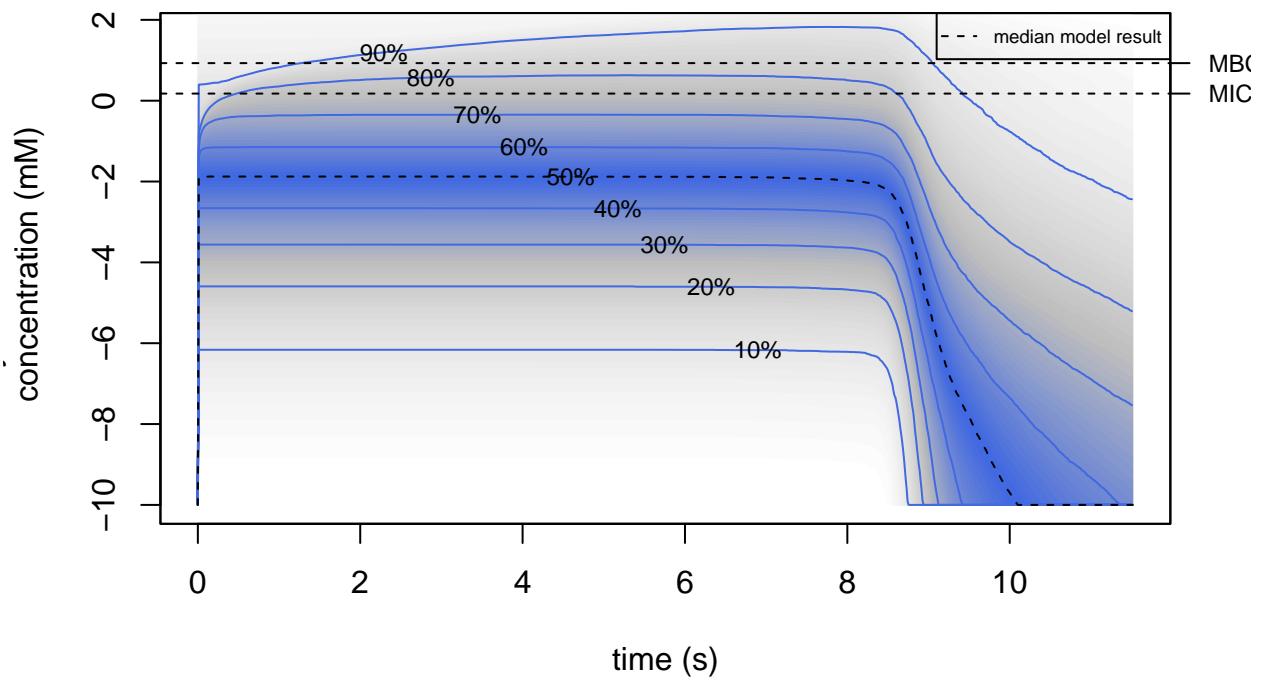
Time series distribution of external 1,3-PDO concentration (mM)



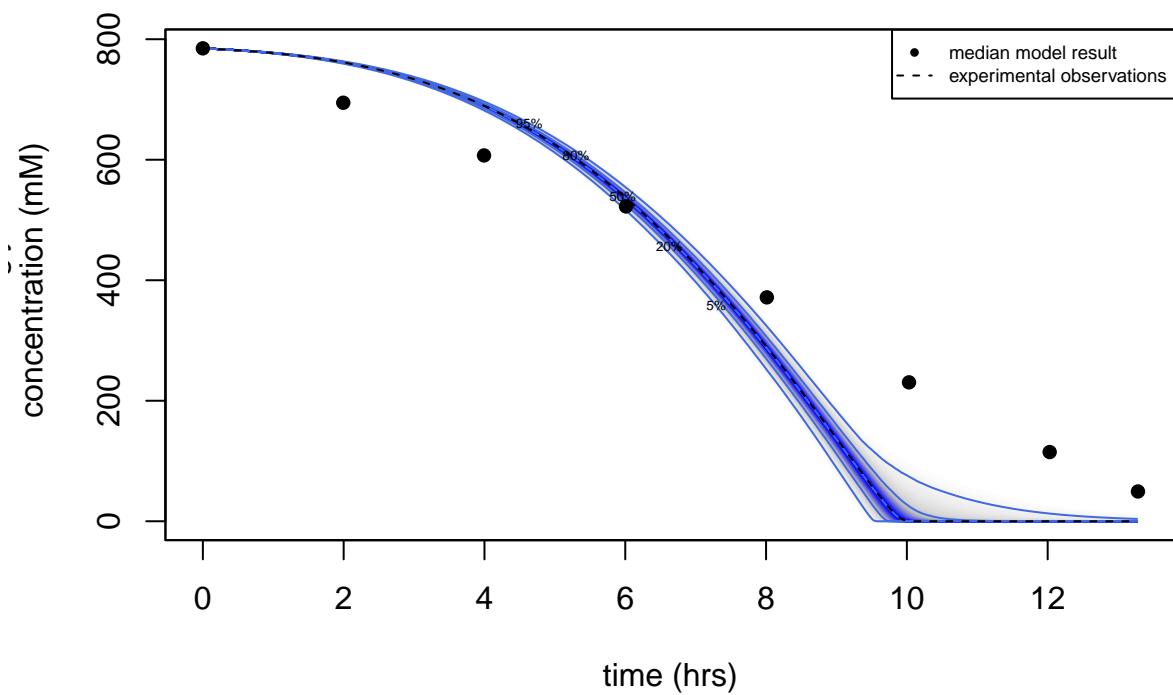
Time series distribution of cytosolic 3–HPA concentration (mM)



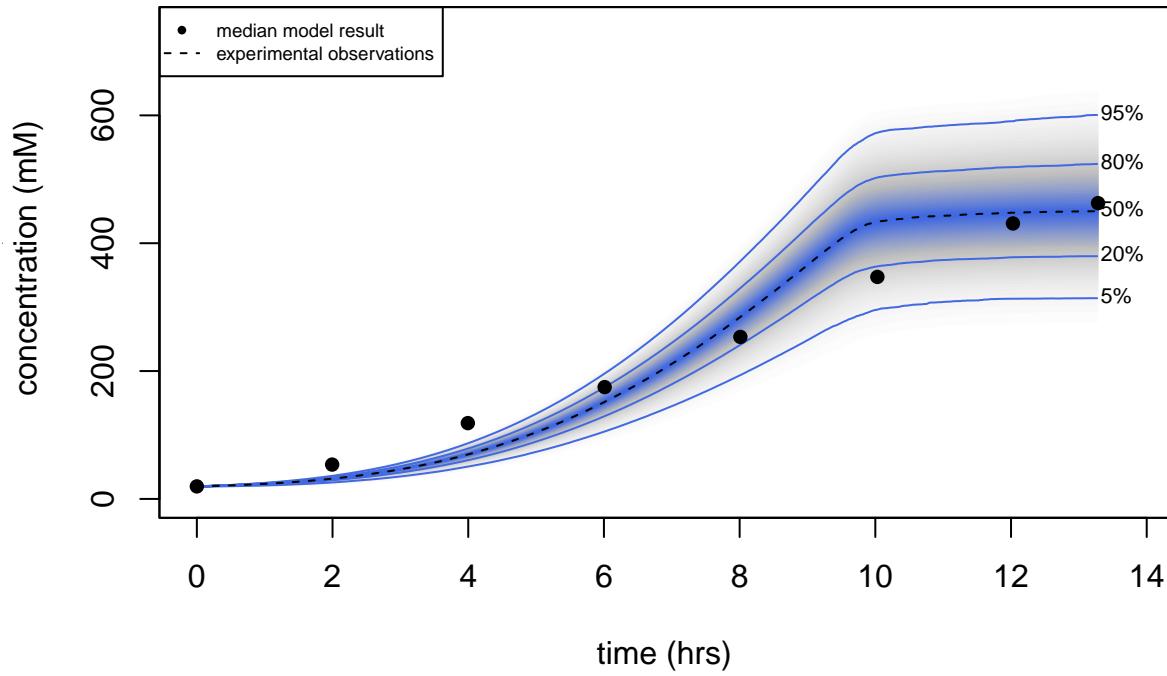
Time series distribution of cytosolic 3–HPA concentration (mM)



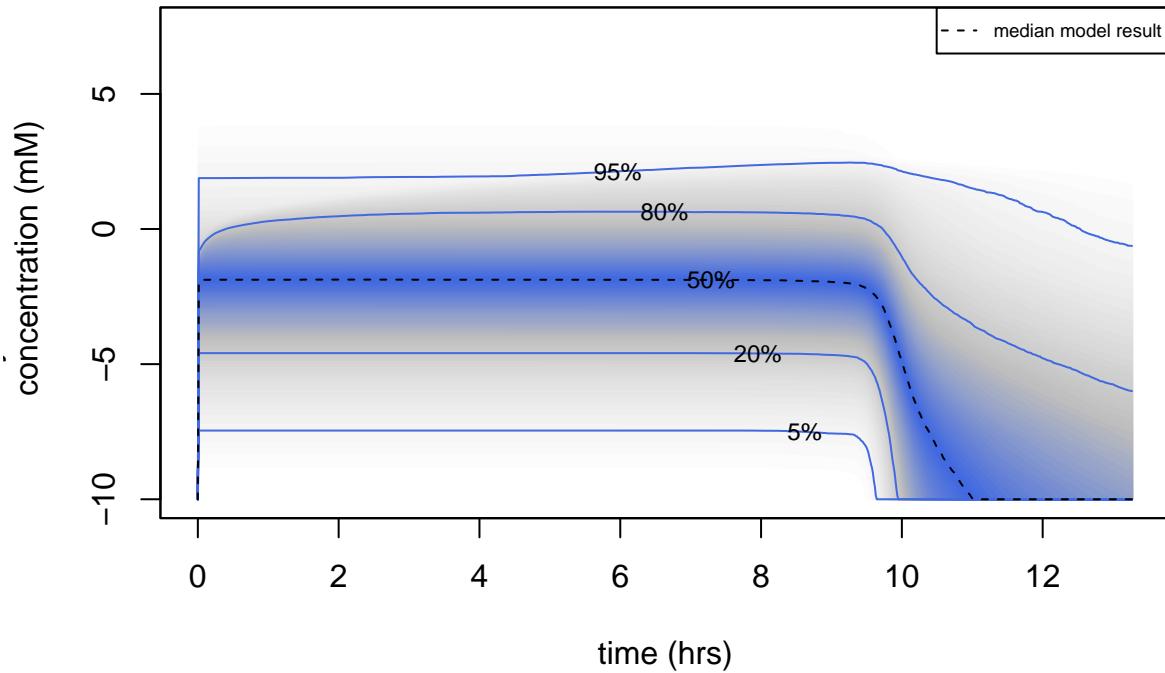
Time series distribution of external glycerol concentration (mM)



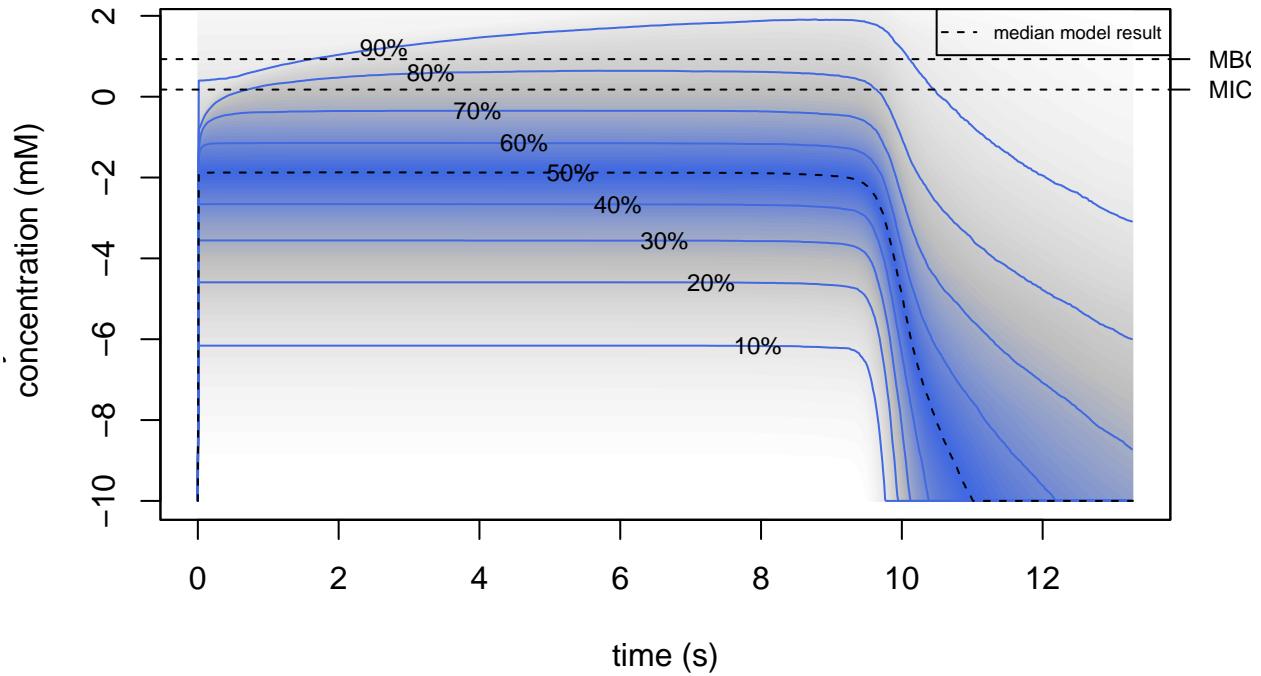
Time series distribution of external 1,3-PDO concentration (mM)



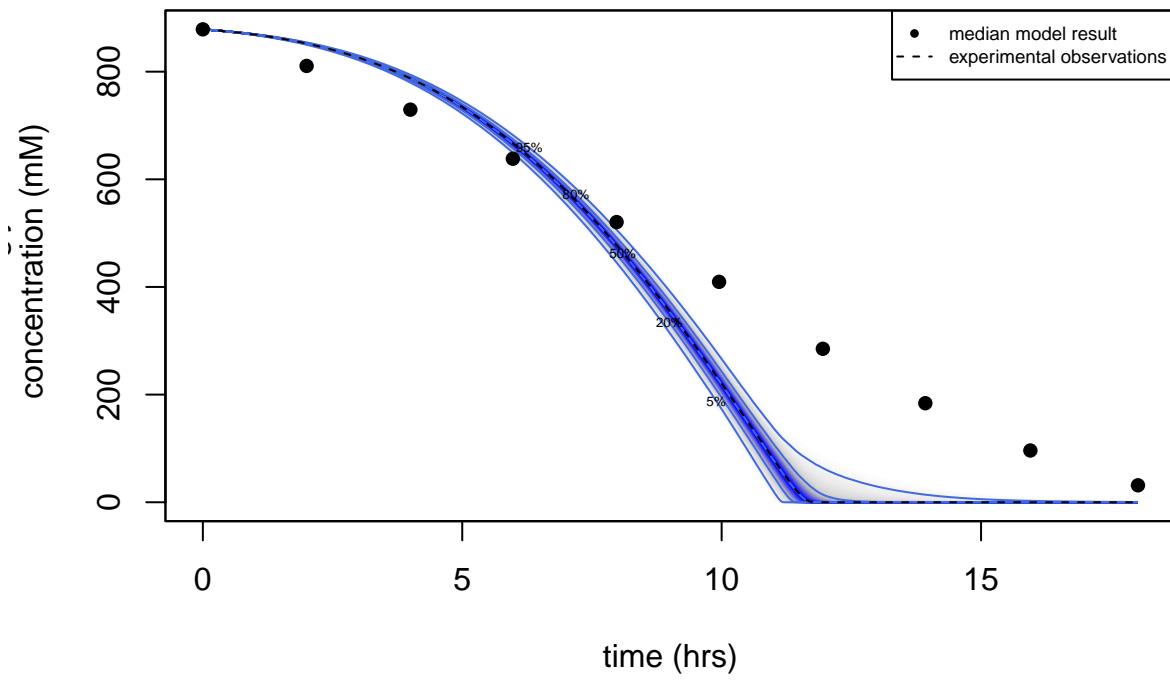
Time series distribution of cytosolic 3–HPA concentration (mM)



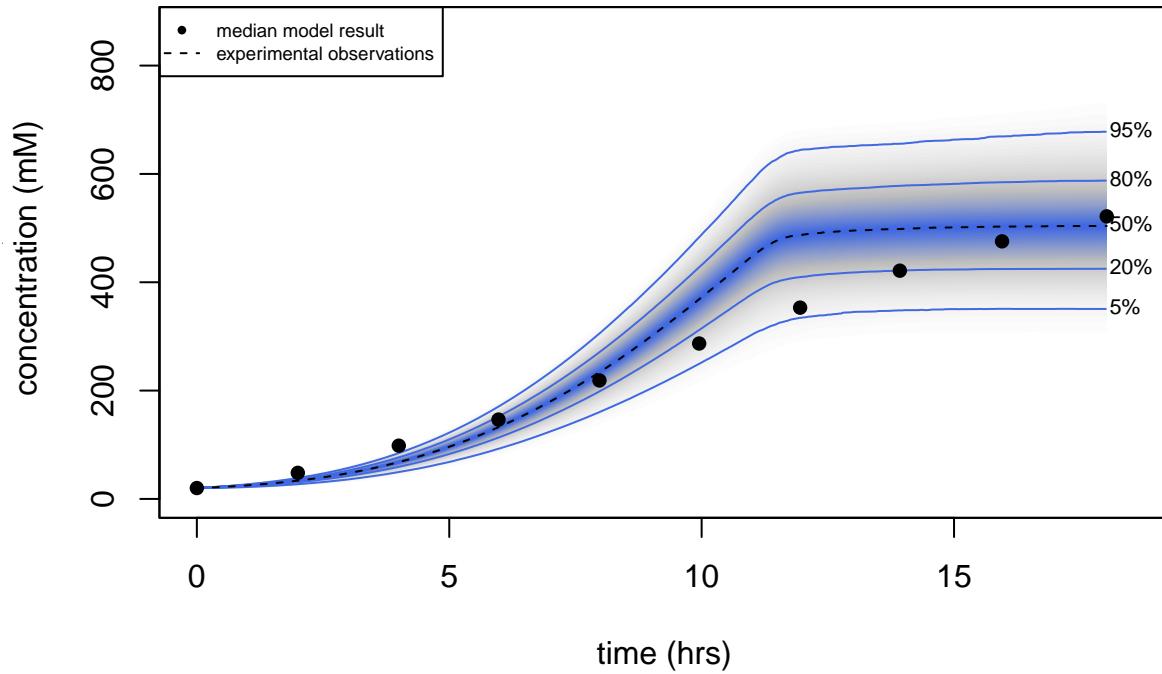
Time series distribution of cytosolic 3–HPA concentration (mM)



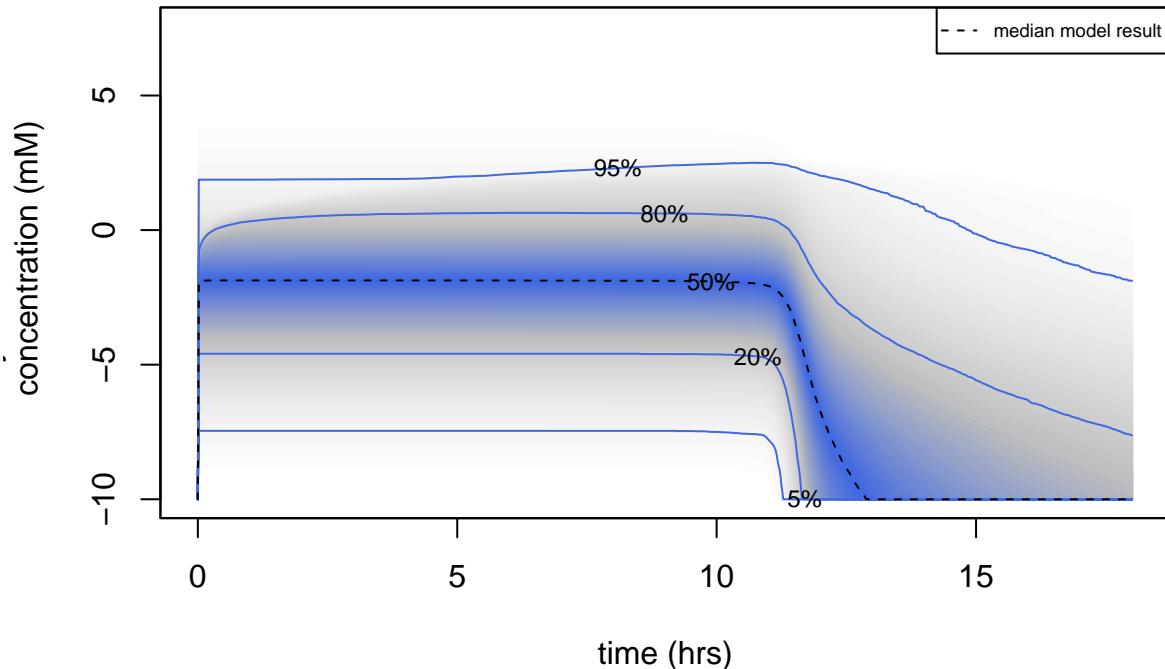
Time series distribution of external glycerol concentration (mM)



Time series distribution of external 1,3-PDO concentration (mM)



Time series distribution of cytosolic 3–HPA concentration (mM)



Time series distribution of cytosolic 3–HPA concentration (mM)

